INVERSE SCATTERING PROBLEM FOR THE SCHRÖDINGER EQUATION IN THREE DIMENSIONS: CONNECTIONS BETWEEN EXACT AND APPROXIMATE METHODS

By

E. Somersalo

G. Beylkin

R. Burridge

and

M. Cheney

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INVERSE SCATTERING PROBLEM FOR THE SCHRÖDINGER EQUATION IN THREE DIMENSIONS: CONNECTIONS BETWEEN EXACT AND APPROXIMATE METHODS

E. SOMERSALO*,
G.BEYLKIN†,
R.BURRIDGE†,
AND
M.CHENEY‡

1. Introduction. In this paper we consider the three-dimensional inverse scattering problem for the Schrödinger equation: the scattering potential is to be reconstructed from the asymptotic amplitude (scattering amplitude) of the outgoing scattering solution of the equation. This nonlinear problem has been approached basically from two directions: one can look for exact inversion methods or one can linearize and then solve the linear problem.

The first direction has been taken by a number of researchers (see [1-6] and references therein). Most of the work, however, suffers from the defect that the methods are numerically intractible. A number of methods, in addition, require assumptions that can only be verified once the inverse problem has been solved.

From the second direction there was a major effort in applications to solve the linearized inverse problem. Solutions of linearized inverse problems are generally easy to compute and are therefore of importance in a variety of fields, which include quantum mechanics, geophysics, medical imaging and non-destructive testing. However, the drawback of using such solutions is that it is not always clear how they are related to the exact solutions.

In this paper we establish connections between the two directions of research outlined above. We show how certain reconstruction formulas arising from the exact inversion theory lead in the first approximation to formulas that are independently obtainable from linearized schemes.

This paper is organized as follows. In Section 2 we modify slightly the trace type formula of Newton [3] and then compare it to the formula obtained from the linearized inverse problem. In Section 3 we consider an inversion method that uses the zero energy solution of the Schrödinger equation. We relate this method to the trace-type formula of Section 2 and explain how it is related to inversion methods of the linear theory. In Section 4 we consider reconstruction formulas at high energies. We show that certain high energy limit theorems are closely related to reconstruction formulas of linear theory.

*Department of Mathematics, University of Helsinki, Hallituskatu 15, 00100 Helsinki, Finland.
†Schlumberger-Doll Research, Old Quarry Road, Ridgefield, CT 06877
‡Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, New York 10012; Permanent address: Rensselaer Polytechnic Institute, Department of Mathematical Sciences, Troy, NY 12181.

2. The trace-type formula and its relation to linearized reconstruction. In a paper on the one-dimensional inverse scattering problem Deift and Trubowitz [7] derive a formula that gives the potential of the Schrödinger equation in terms of the scattering data and the unknown wave function. This formula they call the trace formula. In this section we use the three-dimensional analog of this formula, which we describe as a trace-type formula.

We start by establishing notation. We write the three-dimensional Schrödinger equation as

$$(-\Delta_x + V)\Psi = k^2\Psi, \tag{2-1}$$

Δ_x being the Laplacian, V a real scattering potential which satisfies certain regularity conditions specified later, and $k \in \mathbf{C}$. Let $\Psi^+(k,\theta,x)$ denote the outgoing scattering solution of (2-1) with an incident plane wave and $A(k,\theta',\theta)$ the scattering amplitude such that as $|x| \to \infty$

$$\Psi^+(k,\theta,x) = \mathrm{e}^{\mathrm{i}k\theta\cdot x} + \frac{\mathrm{e}^{\mathrm{i}k|x|}}{|x|}A(k,\theta',\theta) + o\left(|x|^{-1}\right), \tag{2-2}$$

where $\theta' = x/|x|$, $\theta \in \mathbf{S}^2$, $k \in \bar{\mathbf{C}}^+ = \{\mathcal{I}m\, k \geq 0\}$, and $A(k,\theta',\theta)$ is given by

$$A(k,\theta',\theta) = -\frac{1}{4\pi}\int_{\mathbf{R}^3} \mathrm{e}^{-\mathrm{i}k\theta'\cdot x}V(x)\Psi^+(k,\theta,x)dx. \tag{2-3}$$

We also define the incoming solution $\Psi^-(k,\theta,x)$ for $k \in \bar{\mathbf{C}}^- = \{\mathcal{I}m\, k \leq 0\}$ by setting $\Psi^-(k,\theta,x) = \Psi^+(-k,-\theta,x)$. It is well known (see e.g. [14,15]) that $\Psi^+(k,\theta,x)$ and $\Psi^-(k,\theta,x)$ are related on the real axis and the relation involves the scattering amplitude:

$$\Psi^+(k,\theta,x) - \Psi^-(k,\theta,x) = -\frac{k}{2\pi\mathrm{i}}\int_{\mathbf{S}^2} A(k,\theta',\theta)\Psi^-(k,\theta',x)d\theta', \tag{2-4}$$

$k \in \mathbf{R}$. This equation is the key to several approaches to inverse scattering. We use it to derive the following trace-type formula (first derived by Newton, [3]) for the reconstruction of V from A and Ψ^-.

PROPOSITION 2.1. *Let the potential V satisfy the following conditions:*

(1) $V \in L^1 \cap L^2$
(2) $|V(x)|$ and $|\nabla V(x)|$ are bounded above by a function $F(|x|)$ with $\int_0^\infty F(t)dt < \infty$
(3) V produces no bound states.

Then

$$V(x) = \frac{1}{2\pi^2\mathrm{i}}\theta\cdot\nabla_x \int_{-\infty}^{+\infty} kdk \int_{\mathbf{S}^2} d\theta' A(k,\theta',\theta)e^{-\mathrm{i}k\theta\cdot x}\Psi^-(k,\theta',x), \tag{2-5}$$

Proof. See Appendix. The Appendix also includes a modification of (2-5) that applies in the presence of bound states.

We consider the following inverse problem: given the scattering amplitude for *all* energies k, *all* directions of the incident field, and measured at *all* scattered directions, find the potential. Thus, $A(k,\theta',\theta)$ is defined on the space $\mathbf{R}\times\mathbf{S}^2\times\mathbf{S}^2$. We note that in practice scattering data are measured over a finite interval of energies which leads to a bandlimited reconstruction. It is clear that A contains redundant information since A is a function of five variables, whereas V is a function of three only.

In practice redundant scattered data are collected routinely; it is therefore useful to have a reconstruction where all data are involved. This type of redundancy is possible only in the multidimensional case since only then does the count of variables in the scattered data exceed that for the potential.

In the linearized problem the apparent difficulty of dealing with redundant information is taken care of by expressing the inverse Fourier transform on the space $\mathbf{R}\times\mathbf{S}^{n-1}\times\mathbf{S}^{n-1}$ as derived by Burridge and Beylkin in [8]. We have

PROPOSITION 2.2. *Let F be a function on $\mathbf{R}^n$ and $\hat{F}$ its Fourier transform. We assume that F is in a class of functions for which the inverse Fourier transform formula $F(x)=(2\pi)^{-n}\int_{\mathbf{R}^n}\hat{F}(p)e^{ip\cdot x}dp$ holds. Then*

$$F(x)=\frac{1}{4\,(2\pi)^n\,\Omega_{n-1}}\int_{-\infty}^{+\infty}|k|^{n-1}dk\cdot \tag{2-9}$$
$$\int_{\mathbf{S}^{n-1}\times\mathbf{S}^{n-1}}d\theta d\theta'\frac{|\theta-\theta'|^{n-1}W\left(x,\frac{1}{2}|\theta-\theta'|\right)}{\left(1-(\theta\cdot\theta')^2\right)^{(n-3)/2}}\hat{F}\left(k\theta-k\theta'\right)e^{i\left(k\theta-k\theta'\right)\cdot x},$$

where W is an arbitrary function such that

$$\int_0^1 W\left(x,\rho\right)d\rho=1, \tag{2-10}$$

and $\Omega_n=2\pi^{n/2}/\Gamma\left(n/2\right)$ is the surface measure of the unit sphere in $\mathbf{R}^n$.

Specializing this statement to the case of dimension $n=3$ and weight $W=1$, we have

$$F(x)=\frac{1}{64\pi^4}\int_{-\infty}^{+\infty}k^2dk\int_{\mathbf{S}^2\times\mathbf{S}^2}d\theta d\theta'|\theta-\theta'|^2\hat{F}\left(k\theta-k\theta'\right)e^{i\left(k\theta-k\theta'\right)\cdot x}, \tag{2-11}$$

Formula (2-11) was derived independently by a number of researchers (see Rose and Cheney [9] and references therein). Proposition 2.2, in fact, maps the space $\mathbf{R}\times\mathbf{S}^{n-1}\times\mathbf{S}^{n-1}$ onto the ordinary Fourier space.

Linearizing the inverse scattering problem by replacing $\Psi^+(k,\theta,x)$ in (2-3) by its asymptotic form, the incident wave function $e^{ik\theta\cdot x}$, we obtain the Born approximation

$$A_B(k,\theta',\theta) = -\frac{1}{4\pi}\hat{V}(k\theta' - k\theta). \tag{2-12}$$

Thus, if in (2-9) we replace F by V and $\hat{F}$ by A_B, we have a reconstruction formula for V. This suggests that if in (2-9) we replace $\hat{F}$ by A, we should obtain an approximate reconstruction formula. The choice of W affects the spatial resolution of the reconstruction. In this paper we set $W = 1$ and consider the case when the reconstruction formula is based on (2-11).

PROPOSITION 2.3. *The solution V_0 of the linearized inverse scattering problem (an approximation for the potential V) can be expressed as*

$$V_0(x) = -\frac{1}{16\pi^3}\int_{-\infty}^{+\infty} k^2\,dk \int_{S^2\times S^2} d\theta d\theta' |\theta - \theta'|^2 A(k,\theta',\theta) e^{-i(k\theta - k\theta')\cdot x}, \tag{2-13}$$

This formula explicitly uses all the data. In practice the scattering amplitude is measured only over a finite range of energies and some subset of $S^2 \times S^2$. Thus, $k\theta - k\theta'$ will cover some bounded domain in the space of spatial frequencies and, therefore, in practical applications we will obtain a bandlimited reconstruction via (2-13).

We now show that the trace formula (2-5) yields (2-13) as the first approximation. Let us define

$$\phi^-(k,\theta',x) = \Psi^-(k,\theta',x)e^{-ik\theta'\cdot x}. \tag{2-14}$$

PROPOSITION 2.4. *Let the potential V satisfy the conditions of Proposition 2.1. Then*

$$V(x) = -\frac{1}{16\pi^3}\int_{-\infty}^{+\infty} k^2\,dk \int_{S^2\times S^2} d\theta d\theta' \cdot \left[|\theta - \theta'|^2 \phi^-(k,\theta',x) + \frac{2i}{k}\theta\cdot\nabla_x \phi^-(k,\theta',x)\right] A(k,\theta',\theta) e^{-ik(\theta-\theta')\cdot x}. \tag{2-15}$$

Proposition 2.4 follows trivially from Proposition 2.1 if we integrate (2-5) over S^2 and take the gradient inside the integral.

We notice that $\phi^-(k,\theta',x)$ is known to be close to the free space solution, $\phi_0^-(k,\theta',x) = 1$ under a number of conditions. For example, if the potential V is small (weak scattering), then $\phi^-(k,\theta',x)$ is a small perturbation of $\phi_0^-(k,\theta',x)$. Also, if k is large then $\phi^-(k,\theta',x)$ is close to $\phi_0^-(k,\theta',x)$. Substituting ϕ_0^- for ϕ^- into (2-15) we obtain the first approximation of (2-15), which is precisely (2-13). We note that this is the same approximation that was used to obtain (2-12) (and, hence (2-13)) via linearization.

3. A zero energy trace-type formula. In this section we consider an inverse scattering method that uses the zero-energy solution

$$\Psi(x)=\Psi^{+}(0,\theta,x)=\Psi^{-}(0,\theta,x). \tag{3-1}$$

It is clear that this zero energy solution does not depend on θ. It satisfies

$$\Delta_x\Psi(x)=V(x)\Psi(x), \tag{3-2}$$

thus if $\Psi(x)$ is known, the potential $V(x)$ can be recovered via (3-2). We therefore turn our attention to the recovery of $\Psi(x)$ from A.

PROPOSITION 3.1. *Let the potential V satisfy the conditions of Proposition 2.1 and assume that $k=0$ is not an exceptional point. Then*

$$\Psi(x)=1+\frac{1}{4\pi^2}\int_{-\infty}^{+\infty}dk\int_{\mathrm{S}^2}d\theta' A(k,\theta',\theta)\mathrm{e}^{-\mathrm{i}k\theta\cdot x}\Psi^{-}(k,\theta',x). \tag{3-3}$$

or

$$\Psi(x)=1+\frac{1}{16\pi^3}\int_{-\infty}^{+\infty}dk\int_{\mathrm{S}^2\times\mathrm{S}^2}d\theta d\theta' A(k,\theta',\theta)\mathrm{e}^{-\mathrm{i}k\theta\cdot x}\Psi^{-}(k,\theta',x). \tag{3-4}$$

Formula (3-3) was first obtained by Newton in [3]. We note that the right hand side of (3-3) depends on θ while $\Psi(x)$ does not. In this sense it is similar to Newton's "miracle".

The proof of this Proposition comes directly from formula (5-5) of the Appendix, where we set $k=\mathrm{i}\epsilon$, with $\epsilon\to 0$. Since we assume that $k=0$ is not an exceptional point this limit exists. Equation (3-4) is obtained from (3-3) by integration over the unit sphere.

The trace-type formulas of Proposition 3.1 are related to those of Propositions 2.1 and 2.4. To see this let us derive (2-15) from (3-4), for example. We first compute

(3-5)

$$\Delta_x\left[\mathrm{e}^{-\mathrm{i}k(\theta-\theta')\cdot x}\phi^{-}(k,\theta',x)\right]=\mathrm{e}^{-\mathrm{i}k(\theta-\theta')\cdot x}$$
$$\left[-k^2|\theta-\theta'|^2\phi^{-}(k,\theta',x)-2\mathrm{i}k\theta\cdot\nabla_x\phi^{-}(k,\theta',x)+2\mathrm{i}k\theta'\cdot\nabla_x\phi^{-}(k,\theta',x)+\Delta_x\phi^{-}(k,\theta',x)\right].$$

Next we use

$$2\mathrm{i}k\theta'\cdot\nabla_x\phi^{-}(k,\theta',x)+\Delta_x\phi^{-}(k,\theta',x)=V(x)\phi^{-}(k,\theta',x). \tag{3-6}$$

to simplify (3-5):

$$\Delta_x\left[\mathrm{e}^{-\mathrm{i}k(\theta-\theta')\cdot x}\phi^{-}(k,\theta',x)\right]=\Big[-k^2|\theta-\theta'|^2\phi^{-}(k,\theta',x)-2\mathrm{i}k\theta\cdot\nabla_x\phi^{-}(k,\theta',x)+ V(x)\phi^{-}(k,\theta',x)\Big]\mathrm{e}^{-\mathrm{i}k(\theta-\theta')\cdot x}. \tag{3-7}$$

We now substitute (3-4) into (3-2) and compute $\Delta_x\Psi$ using (3-7). We obtain (2-15) and one can see that the first two terms in (3-7) yield the integrand of (2-15).

Interpretation of (3-3),(3-4) and (3-2). Using (2-6) and changing θ, θ' to $-\theta, -\theta'$ we rewrite (3-3) and (3-4) as

$$\Psi(x) = 1 + \frac{1}{4\pi^2} \int_{-\infty}^{+\infty} dk \int_{S^2} d\theta' A(k, \theta, \theta') e^{ik\theta \cdot x} \Psi^-(k, -\theta', x), \tag{3-8}$$

and

$$\Psi(x) = 1 + \frac{1}{16\pi^3} \int_{-\infty}^{+\infty} dk \int_{S^2 \times S^2} d\theta d\theta' A(k, \theta, \theta') e^{ik\theta \cdot x} \Psi^-(k, -\theta', x). \tag{3-9}$$

In the literature devoted to applied linearized inverse scattering theory (especially for acoustic and elastic equations in geophysics and medical imaging) certain terminology has been developed over the years with respect to procedures similar to those contained in formulas (3-8)-(3-9). For example, the computation of the integral $\int_{S^2} d\theta' A(k, \theta, \theta') \Psi^-(k, -\theta', x)$ in (3-8) and (3-9) is called *backpropagation* since this integral is a linear superposition of solutions Ψ^- of (2-1) weighted by the scattering amplitude. The solution $\Psi^-(k, -\theta', x)$ can be thought of as propagating backwards in time. The product of such a backpropagated field and the incident field $e^{ik\theta \cdot x}$ is integrated over all energies k. Formula (3-9), in addition, contains integration (averaging) over all initial directions. After we obtain $\Psi(x)$ for all points x of interest we apply the spatial operator (3-2) to recover V. The use of a spatial operator is called imaging (or an imaging principle) in some applications. All the procedures mentioned above are present in more complicated solutions of the linearized inverse problem for acoustic and elastic media. For such an interpretation see [17] and references therein.

We mention this type of interpretation here because some approximate algorithms (used, for example, in exploration geophysics) were derived heuristically on this basis.

We also note that within the linearized theory reconstruction formulas (2-13) and (3-8) can be interpreted as an inversion of the Radon transform (see e.g. [8]).

4. Reconstructions at fixed energy. In this section we compare some inversion results for fixed energy obtained within the contexts of exact and of linearized approaches. We formulate these results here as a limit as energy goes to infinity. We note that in practice such formulas are used for fixed (but large) energy, the choice of which determines the spatial resolution [10,11].

We start with a high energy result that appears in another form in earlier work but was reformulated and thoroughly investigated by Saitō [12],

PROPOSITION 4.1. *Let the potential V satisfy the inequality*

$$|V(x)| \le C(1 + |x|)^{-\mu},$$

for some constants $C > 0$ and $\mu > 1$. Then

$$\lim_{k\to\infty} k^2 \int_{S^2\times S^2} d\theta d\theta' A(k,\theta',\theta) e^{-ik(\theta-\theta')\cdot x} = -2\pi \int \frac{V(y)}{|x-y|^2}\, dy, \tag{4-1}$$

We can solve equation (4-1) as follows. We denote the left side of (4-1) by $g(x)$. We write the right side of (4-1) as a pseudodifferential operator. Equation (4-1) thus becomes

$$g(x) = -4\pi^3 \mathcal{F}^{-1}\left(|p|^{-1}\hat{V}\right)(x), \tag{4-4}$$

where $\hat{V}$ denotes the Fourier transform of V, p is the Fourier transform variable, and $\mathcal{F}^{-1}$ is the inverse Fourier transform. Inverting this relation we have

$$V(x) = -\frac{1}{4\pi^3}\mathcal{F}^{-1}\left(|p|\hat{g}\right)(x). \tag{4-5}$$

Writing (4-5) out explicitly we have the following formula

$$V(x) = \lim_{k\to\infty} -\frac{k^3}{4\pi^3}\int_{S^2\times S^2} d\theta d\theta' |\theta'-\theta| A(k,\theta',\theta) e^{-ik(\theta-\theta')\cdot x}. \tag{4-2}$$

(The order of limit $k \to \infty$ and the inverse Fourier transform $\mathcal{F}^{-1}$ can be exchanged using standard arguments [13].) Formula (4-2) appears in [11]; it grew out of a formula obtained by Devaney [10].

5. Appendix.

In this appendix we prove Proposition 2.1. We start by defining functions $\Phi^{\pm}(k,\theta,x)$ for $k \in \mathbf{C}^{\pm}$ by setting

$$\Phi^{\pm}(k,\theta,x) = e^{-ik\theta\cdot x}\Psi^{\pm}(k,\theta,x) - 1, \qquad k \in \mathbf{C}^{\pm}. \tag{5-1}$$

We will need the following fact about $\Phi^{\pm}$:

PROPOSITION 5.1. *Due to assumptions on V in Proposition 2.1, $\Phi^{\pm}(k,\theta,x)$ regarded as functions of k are analytic in $\mathbf{C}^{\pm}$ and belong to the Hardy class $\mathbf{H}^2(\mathbf{C}^{\pm})$ and if $k=0$ is not an exceptional point they are continuous in $\bar{\mathbf{C}}^{\pm}$.*

This statement can be proved with minor modifications of the proof of Newton [4]. See also [16] for an equivalent statement with more restrictive assumptions on V.

We now prove Proposition 2.1. Let us define the function $\Phi(k,\theta,x)$ for $k \in \mathbf{C}\backslash\mathbf{R}$ as follows

$$\Phi(k,\theta,x) = \begin{cases} \Phi^{+}(k,\theta,x) & k \in \mathbf{C}^{+}, \\ \Phi^{-}(k,\theta,x) & k \in \mathbf{C}^{-}. \end{cases} \tag{5-2}$$

Let $k \in \mathbf{C}\backslash\mathbf{R}$ and choose $K > |k|$. Then by the Cauchy integral formula we have

(5-3) $$\Phi(k,\theta,x) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_K^+ \cup \Gamma_K^-} \frac{\Phi(k',\theta,x)}{k'-k} dk',$$

where the two disjoint paths are chosen as follows: Γ_K^+ consists of the segment $[-K+i0, K+i0$ and a semicircle of radius K in the upper halfplane connecting K and $-K$. Γ_K^- is chosen similarily in the lower halfplane, and integration over Γ_K^+ (Γ_K^-) is in the positive (i.e. counterclockwise) direction. By the Hardy space property, we may let K go to infinity in (5-3), yielding

(5-4) $$\Phi(k,\theta,x) = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{dk'}{k'-k} \mathrm{e}^{-\mathrm{i}k'\theta\cdot x} \left(\Psi^+(k',\theta,x) - \Psi^-(k',\theta,x)\right).$$

Writing the difference $\Psi^+ - \Psi^-$ in terms of the scattering amplitude by means of (2-4), we have

(5-5) $$\Phi(k,\theta,x) = \frac{1}{4\pi^2} \int_{-\infty}^{+\infty} dk' \int_{\mathrm{S}^2} d\theta' \frac{k'}{k'-k} \mathrm{e}^{-\mathrm{i}k'\theta\cdot x} A(k',\theta',\theta)\Psi^-(k',\theta,x').$$

This equation is, in fact, the Fourier transform of the Marchenko equation of Newton [5].

Next we use the fact that $\Psi^{\pm}$ satisfies the Schrödinger equation; we have from (5-1) for $k \in \mathbf{C}^{\pm}$ that

(5-6) $$V(x) = \mathrm{e}^{-\mathrm{i}k\theta\cdot x}(\Delta_x + k^2 - V)\left(\mathrm{e}^{\mathrm{i}k\theta\cdot x}\Phi(k,\theta,x)\right).$$

Substituting (5-5) as the expression for Φ in (5-6) and evaluating the operator using the identity

(5-7)
$$(\Delta_x+k^2)\left(\mathrm{e}^{\mathrm{i}(k-k')\theta\cdot x}f(x)\right) = \mathrm{e}^{\mathrm{i}(k-k')\theta\cdot x}(\Delta_x+k'^2)f(x) + 2\mathrm{i}(k-k')\mathrm{e}^{\mathrm{i}k\theta\cdot x}\theta\cdot\nabla\left(\mathrm{e}^{-\mathrm{i}k'\theta\cdot x}f(x)\right),$$

which holds for any $f(x)$, we arrive at the representation (2-5).

From this derivation, it is clear that the bound states (i.e., poles of Φ) contribute a finite sum of residues to the right hand side of equation (2-5). More precisely, assume that the system has N bound states corresponding to values $k = \pm\mathrm{i}\kappa_1, \ldots, \pm\mathrm{i}\kappa_N$ with residues

(5-8) $$\mathrm{Res}\,\Phi(\pm\mathrm{i}\kappa_j,\theta,x) = \pm\frac{1}{2\mathrm{i}\kappa_j}\mathrm{e}^{\pm\kappa_j\theta\cdot x}\sum_{m=1}^{m=d_j} \mathrm{Y}_j^m(\mp\theta)u_j^m(x).$$

Here $\{u_j^m(x)\}_{m=1}^{m=d_j}$ is a normalized set of eigenfunctions of the Schrödinger operator, d_j is the dimension of the eigenspace corresponding to $\mathrm{i}\kappa_j$ and Y_j^m's are given by

(5-9) $$\mathrm{Y}_j^m(\theta) = \int \mathrm{e}^{\kappa_j\theta\cdot x}V(x)u_j^m(x)dx.$$

Hence, in the presence of bound states (5-5) should be completed with an additional term

$$\sum_{j=1}^{j=N} \frac{\text{Res } \Phi(\pm i\kappa_j, \theta, x)}{\pm i\kappa_j - k} \tag{5-10}$$

and the equation (2-5) should be changed correspondingly. For more details on the treatment of bound states see [4,6].

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